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Comment on gmd-2021-211

David Burdige (Referee)

Referee comment on "RADIv1: a non-steady-state early diagenetic model for ocean sediments in Julia and MATLAB/GNU Octave" by Olivier Sulpis et al., Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2021-211-RC2>, 2021

In this manuscript Sulpis et al. describe a diagenetic model for marine sediments targeted for the study of deep-sea sediments (RADI). Many aspects of this model look like a number of other models that have been previously published, although there are two aspects of this work that stand out. The first is that the model incorporates a more complex (and presumably realistic) representation of carbonate dissolution kinetics, based on recent studies from the USC and CalTech groups. This is an important addition for a number of reasons and warrants eventual publication of this work.

The second is that the model is explicitly discussed in the context of its ability to look at time-dependent problems. Strictly speaking, this is not exactly new since other models out there (e.g., CANDI) can, in principle, also be used to examine time-dependent problems. However, these models generally are not used in this fashion and the work shown here presents some interesting observations based on time-dependent simulations using RADI.

A concern I have, though, about the model is that they use total alkalinity and total DIC as solute variables, rather than calculating them from individual chemical components (I know this is touted as an advantage of this model, but I'm not as convinced that it really is). Given that a major thrust of this work is examining carbonate dissolution in deep-sea sediments this seems like a possible problem. Rather than calculating $[H^+]$ and $[CO_3^{2-}]$ from Alk and DIC profiles (see line 297) wouldn't it make more sense to model H^+ and carbonate (or bicarbonate) concentrations directly in the model and then calculate alkalinity and DIC depth profiles at the end of each time step. Such a model would be just as easy to use as RADI is in terms of comparing model results with field observations and would likely be more accurate. This would probably also require the addition of an equation for borate in the model, but that would be an easy addition (see, for example, the approaches described in Hoffmann et al. [*Biogeosci.* 5, 227-251, 2008] and Faber et al. [*Biogeosci.* 9, 4087-4097, 2012]).

Maybe I'm missing something, but since one of the major efforts here is to more realistically quantify carbonate dissolution in early diagenetic models the approach taken in RADI to "directly" model Alkalinity and DIC as solute variables seems like it adds unnecessary uncertainty. It also requires that they use the bicarbonate diffusion coefficient for DIC and alkalinity (line 395), which adds further uncertainty in the calculation of carbonate ion concentration gradients and fluxes near the sediment surface, which is where most calcium carbonate dissolves in the deep sea.

I also have a number of other questions and smaller concerns about this work. Note that in the rest of this review, the numbers in parentheses refer to line numbers.

- (130-1) – Just so I'm clear, the "diagenetic equations" in RADI are still differential equations (also see the next comment).
- (132) – How exactly does RADI compute "the concentrations of a set of solids and solutes at each time step"? This should be briefly discussed here and perhaps presented in a bit more detail in the supporting information section. Also, in addition to describing these equations part-by-part in the text it might be nice to present some sort of summary of the complete equations in the supporting information section. Perhaps only modeling "geeks" like me would want to see this, but I think it would be good for this to be available, should any reader be so interested in seeing this information.
- (181) – Why and how is *Clay* being modeled here? This is never really discussed (unless I missed it).
- (228) - What exactly is meant by "the reactivities decline with depth"? I'm assuming the k 's in eqn. (4) are constants for a given site (since based on eqns. (7a) and (7b) they only depend on the carbon rain rate to the sediment), so the overall rate of organic matter degradation at any given site should decrease with depth solely because of changes with depth in the quantity of organic matter and the relative proportions of fast and slow decay materials that are present. Am I missing something here?
- (250) – Is there a subscript "z" missing for the k on this line?
- (268) – "This scheme ..." - I would think that the way alkalinity and DIC are modeled in RADI will also make it difficult to apply this model to coastal and anoxic sediments.
- (299) – How are the concentrations of fluoride, borate and silicate obtained?
- (307) – It's not clear to me how the reaction order (η) implicitly accounts for each carbonate mineral's specific surface area. The discussion later on only talks about how the reaction order varies with Ω .
- In the caption to Fig. 2 it states that calcite and aragonite dissolution rates are based on eqns. (8) and (9) but it isn't until you read a little further that you learn that η is actually a complex function of Ω (starting on line 334). It might be good to at least mention this in the figure caption.
- Fig. 4 has two different types of symbols in the O_2 profiles. I think I figured out the differences from reading the text (lines 547-548), but this should be clarified in the figure legend and/or caption.
- (583) – "in the laboratory" but on-board ship? Please clarify.
- (704) - Will tides in the deep sea (water depth 4370 at station #W-2) really generate this large a change in DBL thickness (i.e., from 0.5 to 3.5 mm)?
- (715) – Tides affect both the concentration gradient at the sediment water interface as well as the thickness of the DBL, so the combined effects should then impact the benthic flux. Do these two factors reinforce one another, cancel each other out, or do something in-between? Some of these issues are alluded to indirectly in the next section (4.3), but I wonder if this is worth looking at and/or considering here more

explicitly.

- (753) – I would say “a 5-fold decrease in δ ”.
- (760-1) – “... the quick adjustment of porewater concentrations to the new diffusive boundary layer ...” – Might it be worth showing these profiles (perhaps in the supporting information section)?
- 9 – Please define which color goes with which solute. I’m assuming blue is oxygen, but this (and the other colors) should be explicitly labelled.
- (781) – I think that trying to model carbon isotopes from POC degradation will be challenging if you use a reactive continuum approach, even if this approach is more appropriate for many studies. In part, that is why we use a similar “multi-G” approach to the one used here in our work modeling POC, DIC and DOC degradation in sediments (both total C, ^{13}C and ^{14}C).
- (787) – As noted above, I wonder if applications of the RADI model to coastal sediments will be difficult given the way alkalinity and DIC are being modelled here.

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